Fundamentals of modelling CO2 movement underground

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Fundamentals of Modelling CO_2 Movement underground

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Fundamentals of Modelling CO_2 Movement Underground

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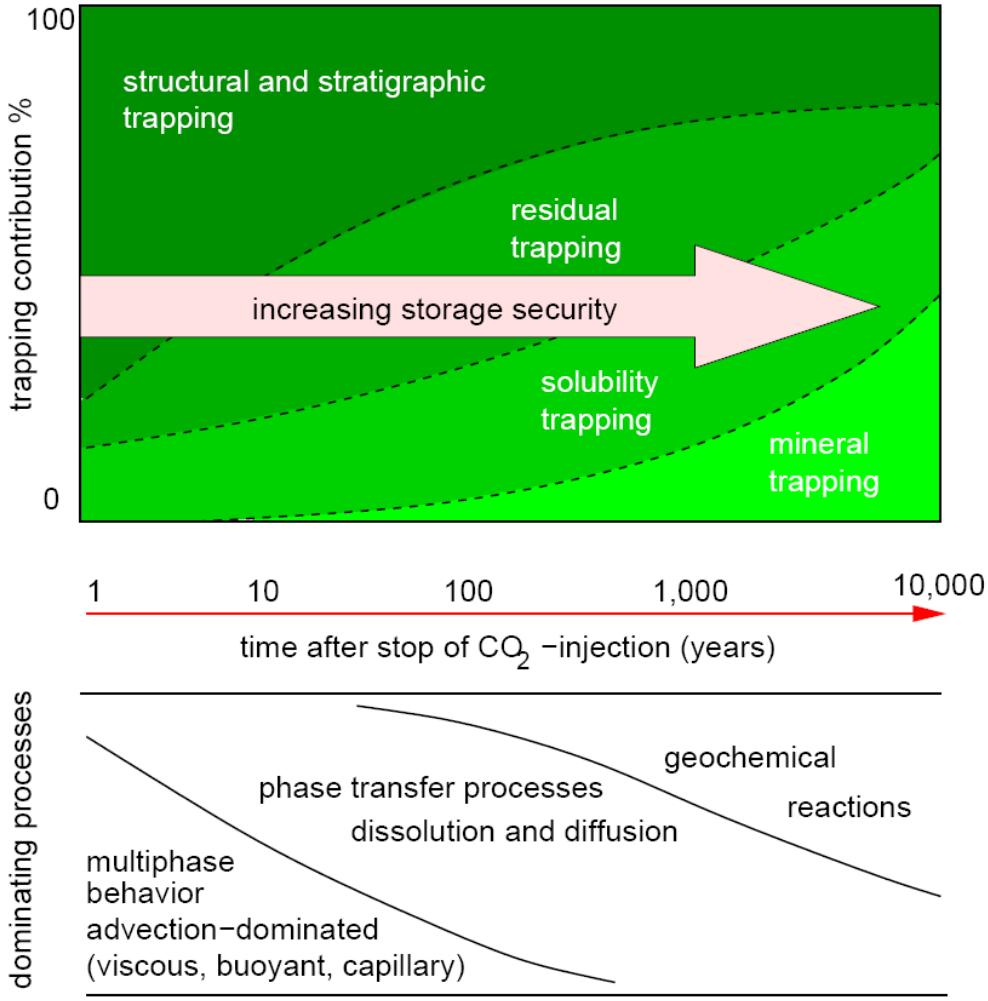
Dynamic Modeling General Objectives

- Capacity Estimation
  - How much CO_2 can we store?
  - Where will the CO_2 flow (CO_2 distribution)?
  - How will the CO_2 partition? (free phase, dissolved, mineral bound)
  - How will the CO_2 distribution evolve with time?
- Formation Injectivity
  - How fast can the CO_2 be injected?
  - In what locations and how (well placement, well type)?
- Storage Integrity
  - Vertical leakage (through wells and faults)
  - Lateral leakage (out of pattern migration)

General considerations of modelling CO_2 injection in saline aquifers

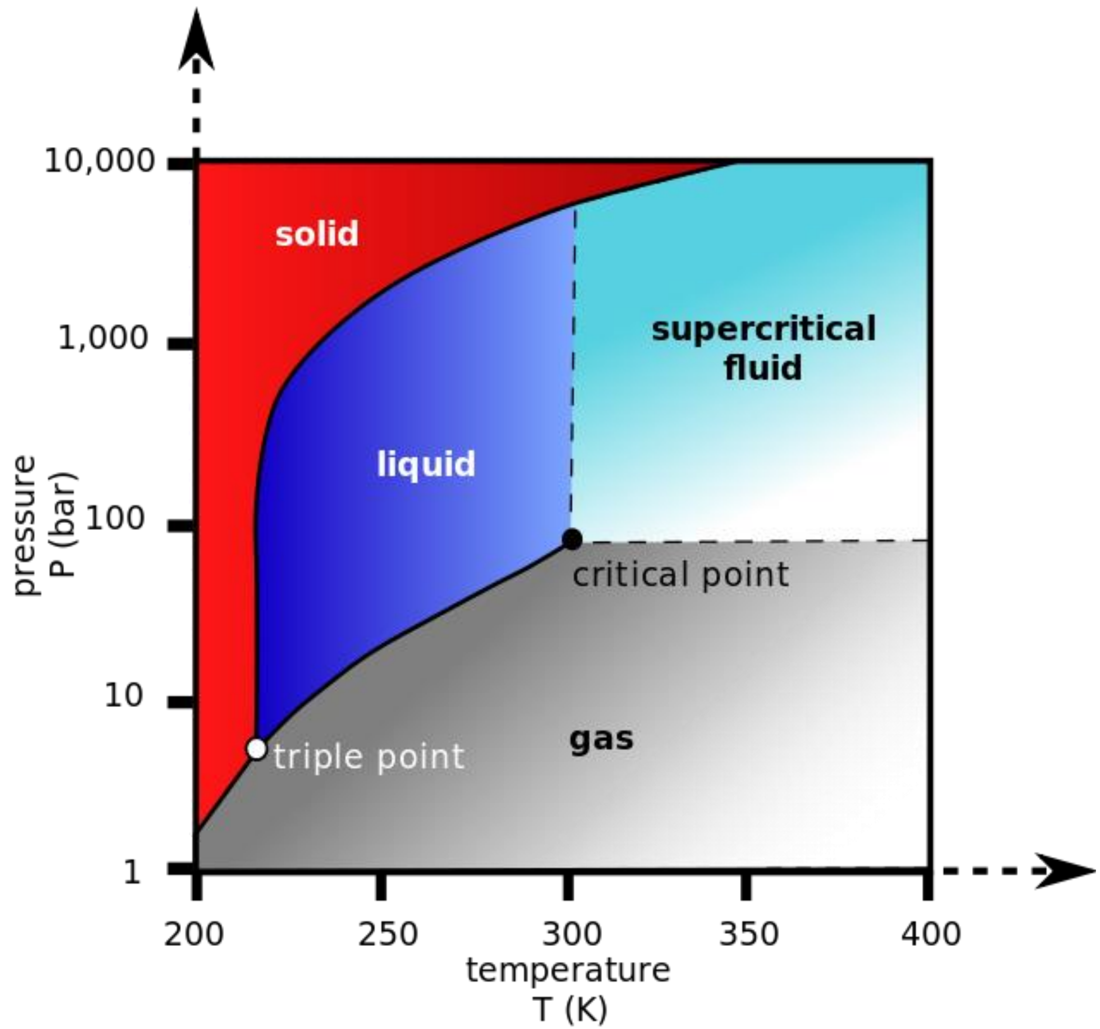
- Two-phase flow (simpler)
- Relative permeability and capillary pressure (hysteresis)
- Buoyant convection (gravity and viscosity instability)
- Phase partitioning
- Thermal effects
- Geochemical interactions
- Geomechanical responses

Geophysical processes: time dependency



IPCC, 2005

Phase Diagram of CO_2



The properties under standard condition at 1.013 bar and 0 °C are:

- Mol. weight: 44.010 g/mol
- Sp. gravity to air: 1.529
- Density: 1.95 kg/m^3

Critical properties:

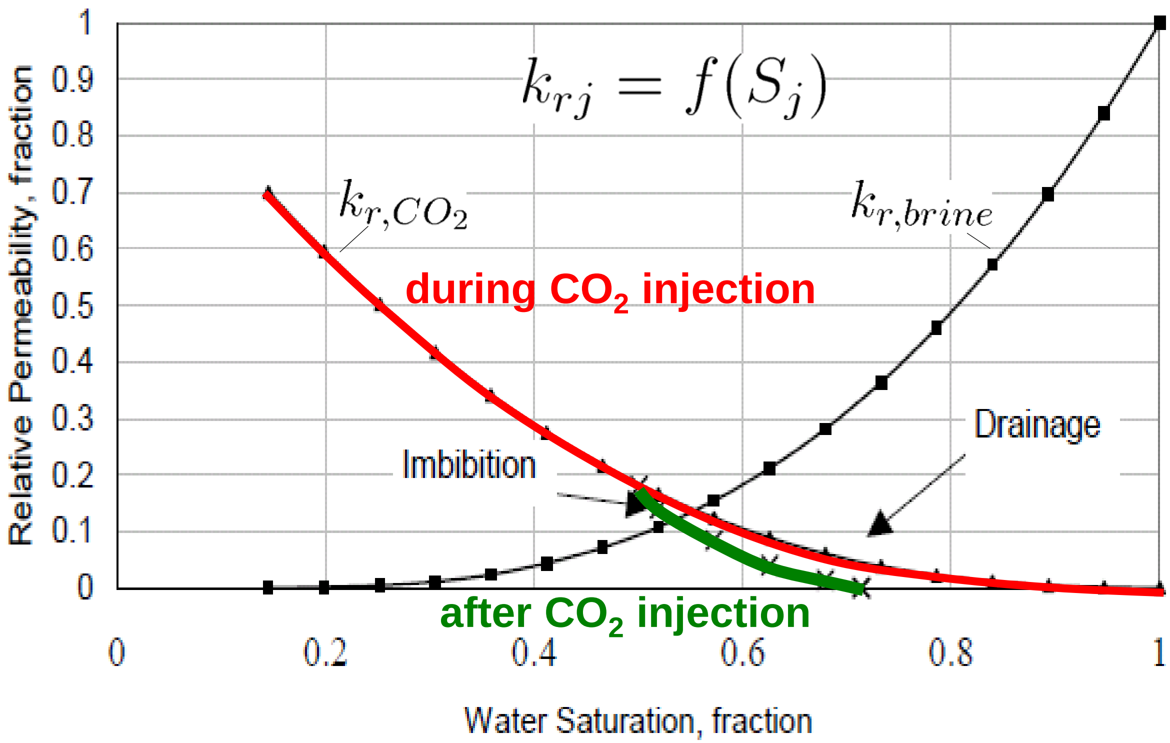
- Tc: 31,05 °C
- Pc: 73.9 bar
- Vc: 94 cm^3/mol

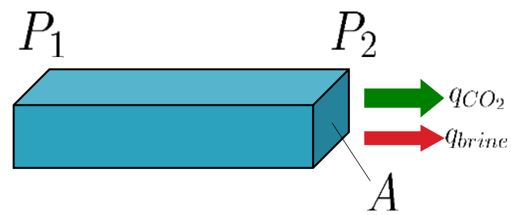
Triple point:

- Ttr: - 56,6 °C
- Ptr: 5.10 bar

Multiphase flow: relative permeability

Hysteresis is important for residual phase trapping





$$\frac{q_j}{A} = -\frac{k_{rj} k}{\mu_j} \nabla P_j$$

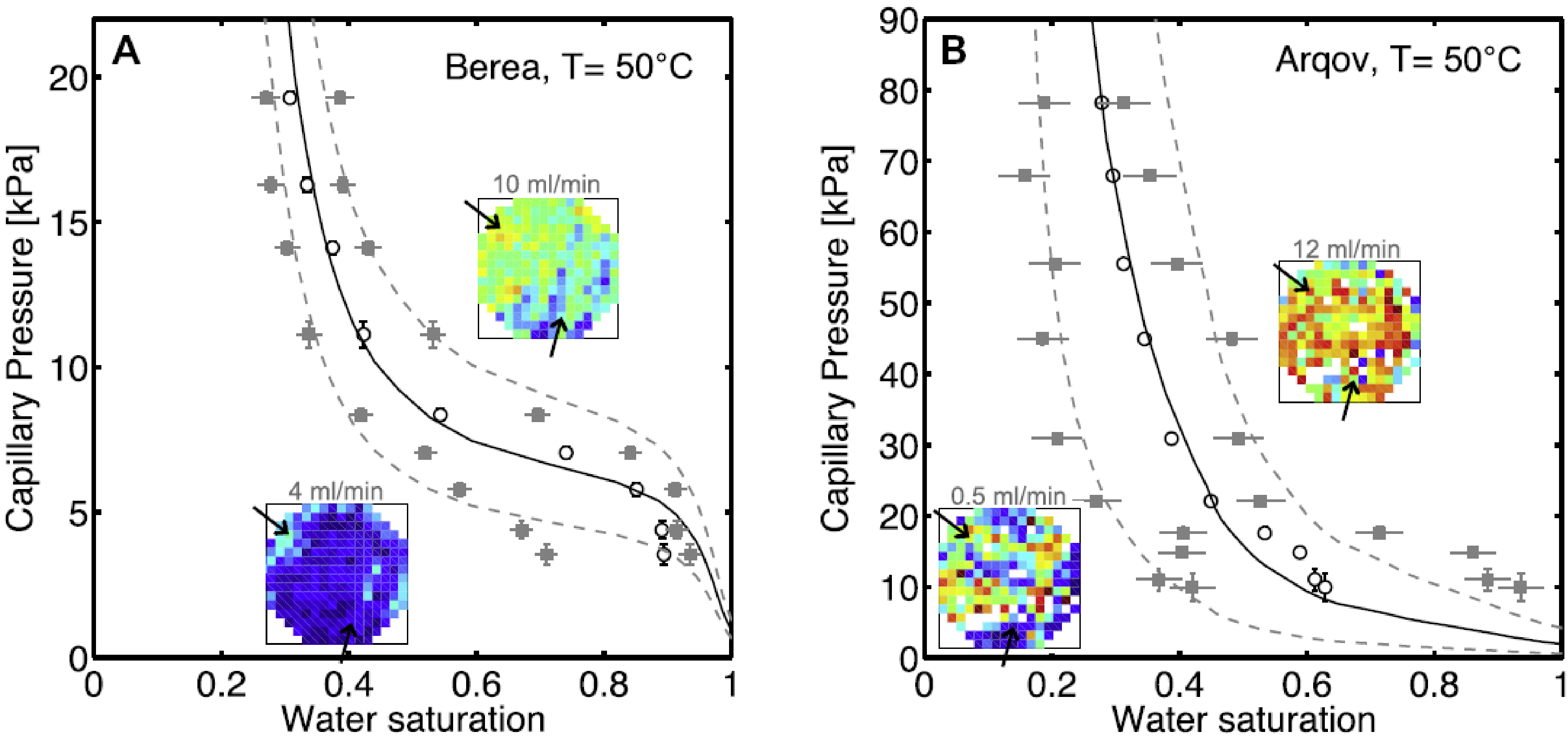
$$j = \mathrm{CO_2} \ or \ \mathrm{brine}$$

$$k_{rj} = f(S_j)$$

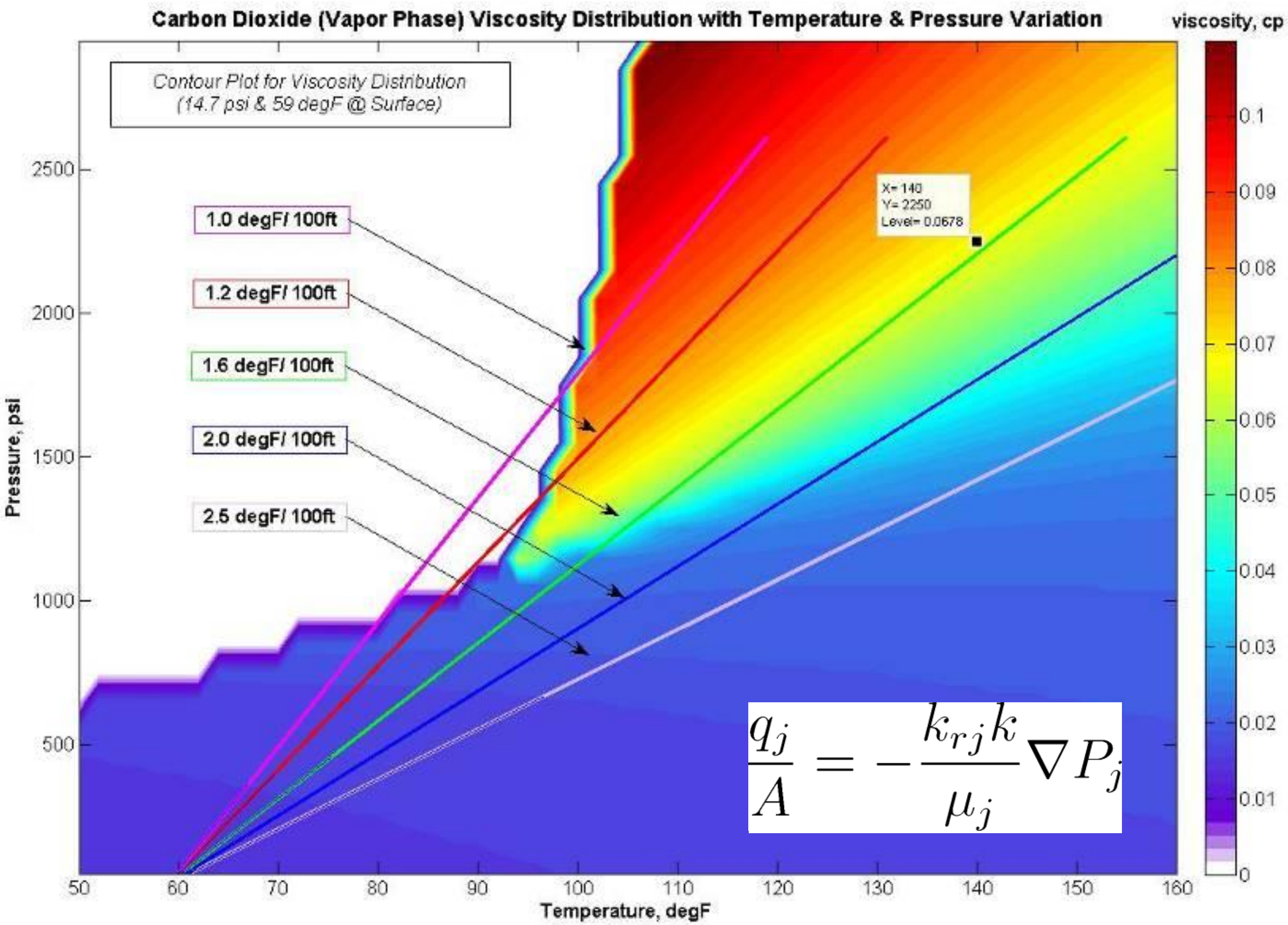
Drainage: CO_2 displaces brine

Imbibition: brine displaces CO_2

Multiphase flow: capillary pressure

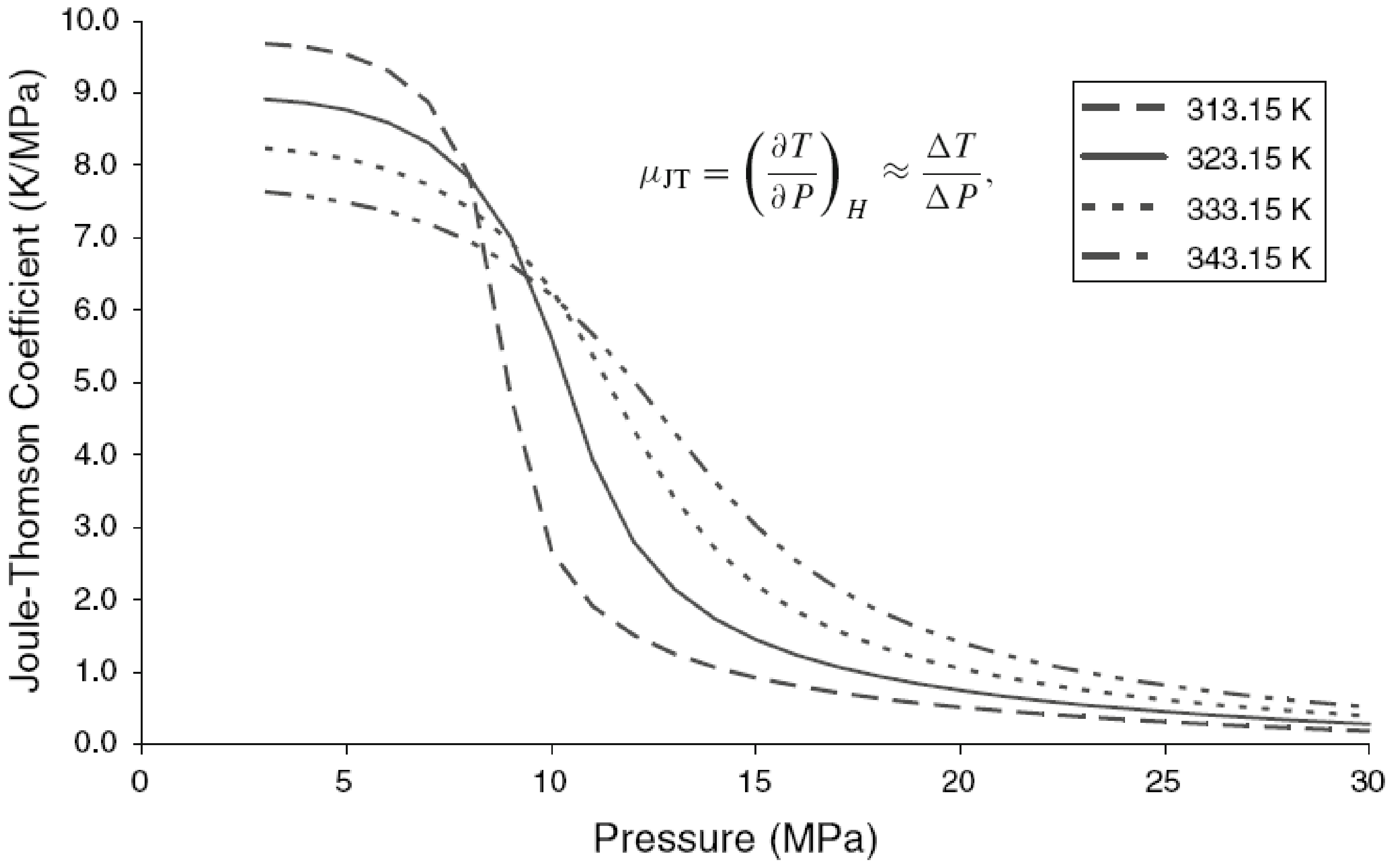


Fluid Properties: Viscosity



Non-isothermal effects

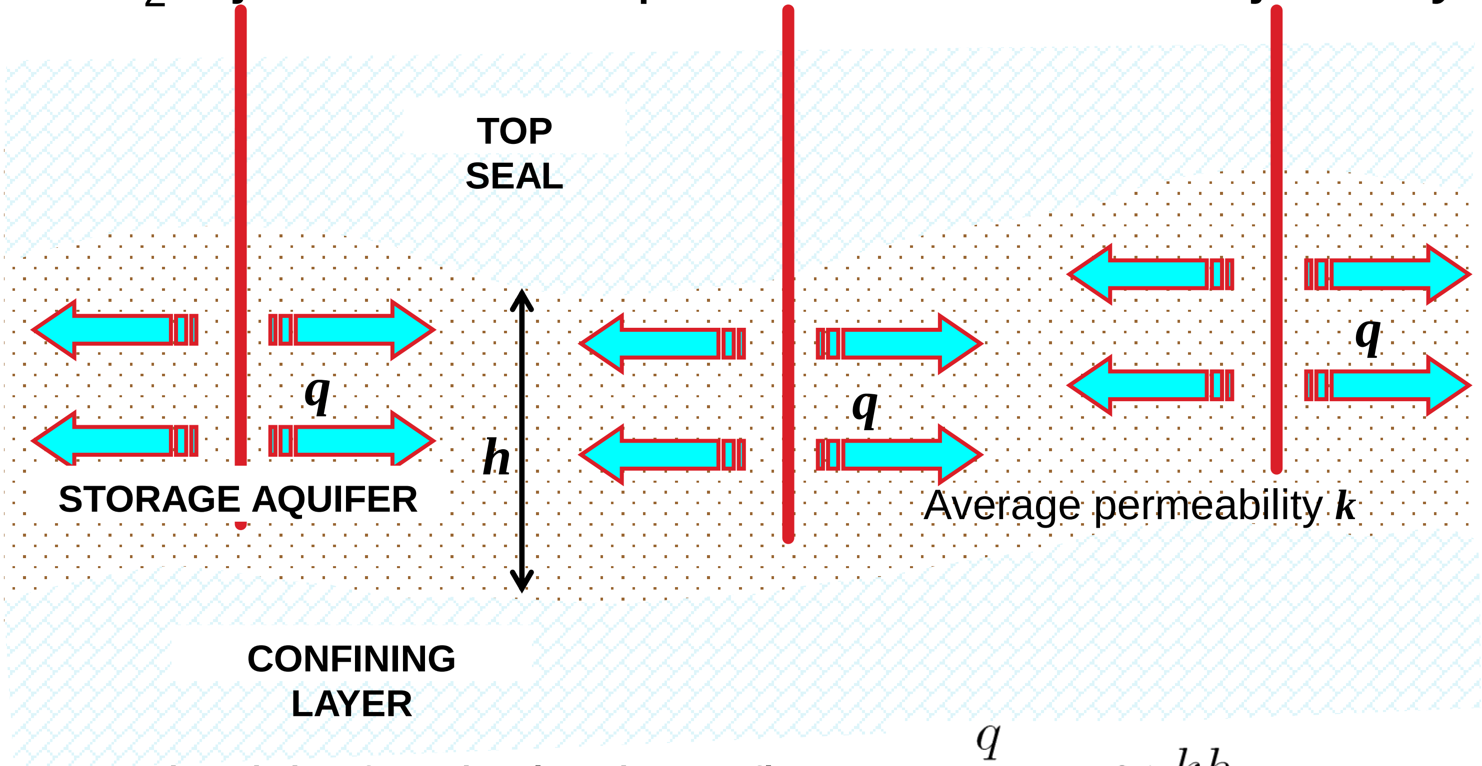
Joule-Thomson effect



NIST Webbook

Analytical Model: Injectivity

CO_2 injection rate depends on formation injectivity



Injectivity for single phase flow $\frac{q}{P_{bh} - \bar{P}} \sim kh$

Injectivity for CO_2 storage *More complicated!*

Analytical Model: Injectivity

Injectivity index depends on formation kh and CO_2 properties

$$II \equiv \frac{q}{\left(P_{bh} - \bar{P}\right)} = 2\pi \frac{kh}{\mu\left(\ln \frac{r_e}{r_w} - \frac{3}{4} + S\right)}$$

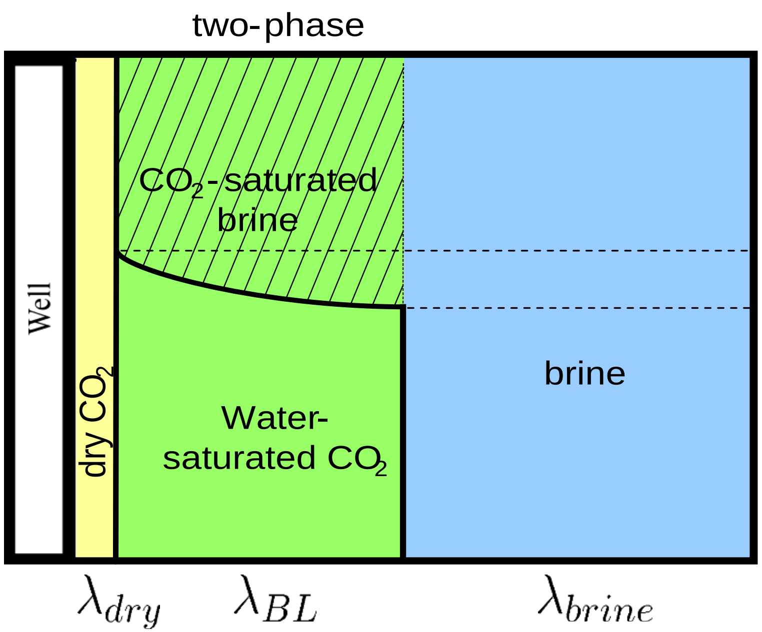
Radial flow
Steady-state
Single phase

$$P_{bh} - P(r) = \frac{q\mu}{2\pi kh}\left(\ln\left(\frac{r}{r_w}\right) + S\right)$$

Where,
II = Injectivity index (single phase flow)
q = CO_2 injection rate @ reservoir conditions
S = skin factor ($-4 < S < 10$)
r_e = aquifer radius
r_w = well radius
μ = brine viscosity
P_{bh} = bottom hole pressure

Analytical Model: Injectivity

Adjust Injectivity index for multiphase flow effects (CO_2 displacing brine)



Rough estimate

$$\lambda_{eff} \approx \frac{\lambda_{brine}}{2} = \frac{1}{2\mu_{brine}}$$

$$\frac{1}{\lambda_{eff}} \sim \frac{1}{\lambda_{dry}} + \frac{1}{\lambda_{BL}} + \frac{1}{\lambda_{brine}}$$

Injectivity index (**two** phase flow)

$$II_{eff} \equiv \frac{q}{P_{bh} - \bar{P}} = 2\pi \frac{kh\lambda_{eff}}{\ln \frac{r_e}{r_w} - \frac{3}{4} + S}$$

Analytical Model: Injectivity

How to use the Injectivity Equation?

$$II_{eff} \equiv \frac{q}{P_{bh}-\bar{P}} = 2\pi \frac{kh\lambda_{eff}}{\ln\frac{r_e}{r_w}-\frac{3}{4}+S}$$

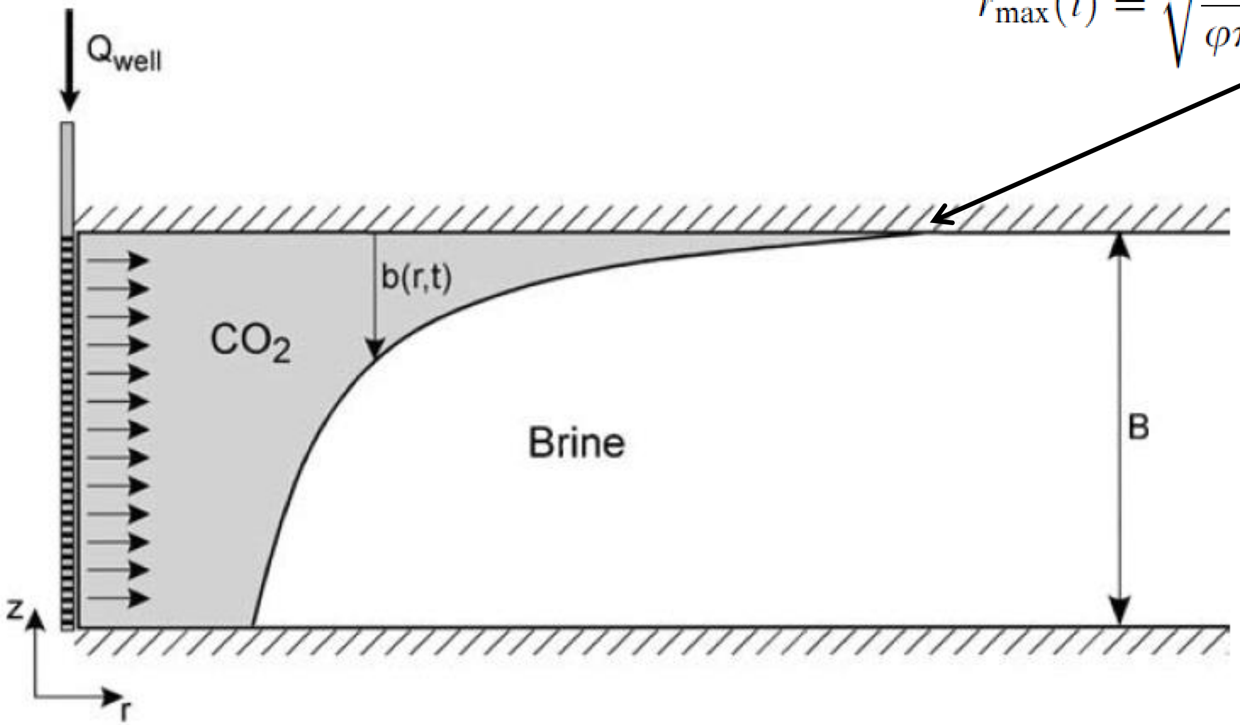
- What we know:
  - q, k, h, r_{e}, r_{w}, S, μ, P
- What can be estimated:
  - Bottom hole pressure (Must be less than fracture pressure)

$$P_{bh} < \quad P_{frac} \approx 0.7\frac{\text{psi}}{\text{ft}} \times z = 16\frac{\text{MPa}}{\text{km}} \times z$$

- If average formation pressure increases during injection, then rate of injection decreases during storage.
- Injection of cold CO_2 can reduce the fracture pressure.

Shape and areal extent of the CO_2 plume

$$r_{\max}(t) = \sqrt{\frac{\lambda_c Q t}{\varphi \pi \lambda_w B}} = C_{\max}\sqrt{t},$$



$\lambda_c / \lambda_w = 10$

Q : m^3/day

t : day

B : m

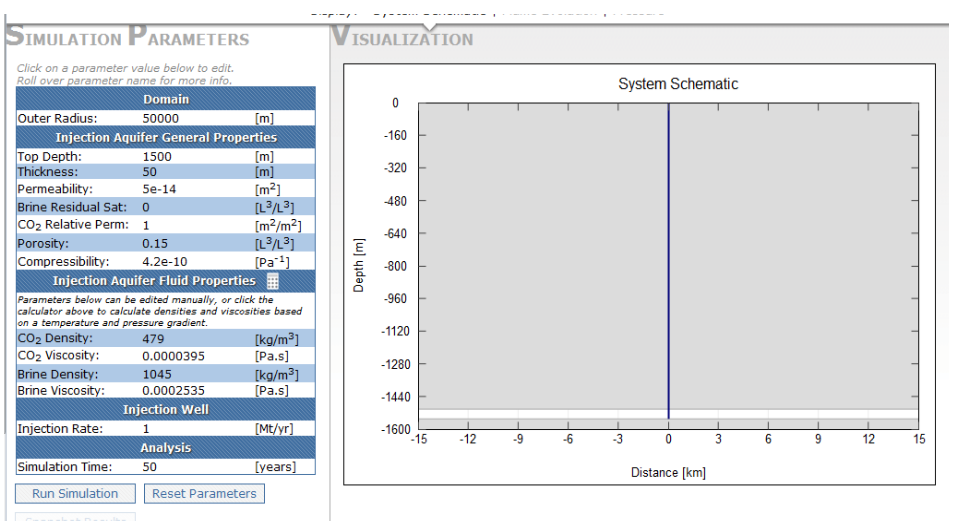
*****

r : m

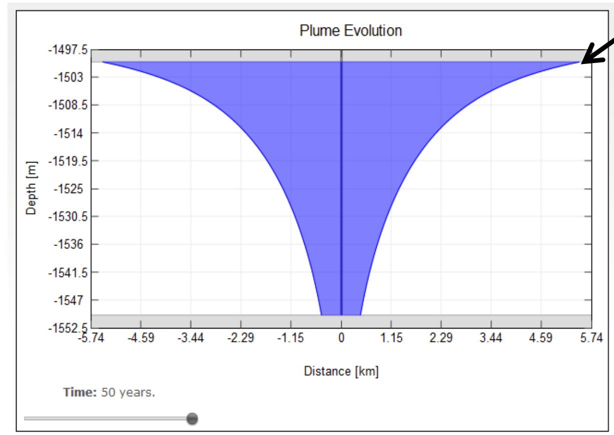
Nordbotten et al., 2005

Shape and areal extent of the CO_2 plume

Useful online tool

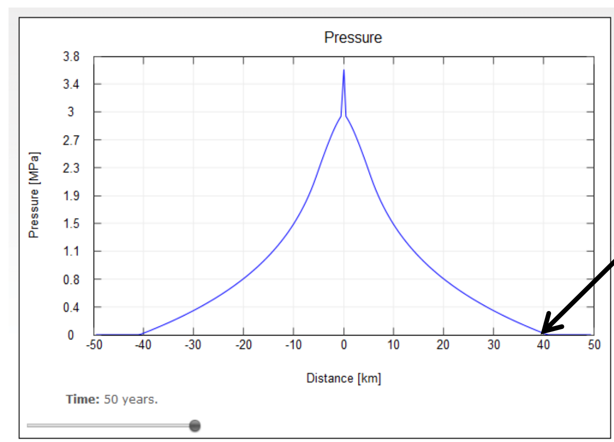


6.7 km



Pressure is a diffusive property and travels faster in the formation

40 km



http://monty.princeton.edu/CO2interface/

Numerical modelling

- Same numerical tools used in the oil industry can be used to simulate CO_2 injection in saline aquifers.
- Proper gridding of reservoir in radial and vertical directions is required, with finer grid resolution close to wellbores and at the top of flow units.
- Upward flow might be exaggerated if aspect ratio of grid is large.
- Both black-oil and compositional models may be used to account for mutual dissolution of CO_2 and brine.
- Mass transfer with reservoir brine is not traditionally included in simulation tools.
- New PVT models have been developed for compositional simutations.

Property (PVT) model

- Cubic EOS (Equations of State) are not able to properly model the compositional properties of the CO_2-brine system.
- Further improvement has been made to allow for the calculation of the mutual dissolution of the water phase (brine) and gaseous phase (CO_2) without using cubic EOS.
- The solubility is obtained by applying the thermodynamic equilibrium for which fugacity of CO_2 in gaseous phase is evaluated based on a cubic EOS (e.g. Peng and Robinson, 1976).
- Fugacity of CO_2 in aqueous phase is calculated based on Henry's law: $f_{CO2} = x_{CO2} * H_{CO2}$

  where x_{CO2} = mole fraction of CO_2 in aquous phase

  $H_{CO2} =$ CO_2 Henry's constant

- Thermodynamic equilibrium is applied to model H_2O vaporization in gaseous phase for which the fugacity of H_2O in gaseous phase is calculated based on the cubic EOS (CMG-GEM, 2012).

Numerical modelling: commonly used codes

	CODES	APPLICATIONS
Fluid Dynamics	GEM, ECLIPSE compositional (E300), TOUGH2, ECO2	Multiphase flow, reservoir system dynamics, plume evolution, storage capacity, CO_2 leakage
Geochemistry	TOUGHREACT, UTCHEM, PHREEQC, Retraso	Fluid-rock interactions, mineral trapping, seal integrity, natural CO_2 analogs
Geomechanics	TOUGH-FLAC, CodeBright	Stress-strain and leakage analysis through seals and faults

Numerical modelling: practical example

Kumar, a., et al, 2004, “Reservoir simulation of CO2 storage in deep saline aquifers”, The university of Texas at Austin, SPE 89343

Evaluate: 1) Pore-level trapping of the CO_2-rich gas phase within the formation
2) Dissolution into brine in the aquifer; and
3) Precipitation of dissolved CO_2 as a mineral, e.g. calcite

Principal petrophysical parameters:

1) Relative permeability (including hysteresis)
2) Residual saturation of non-wetting phase

Used Computer Modeling Group (CMG-GEM)

Numerical modelling: practical example

Simulation Input

Aquifer Properties	
Length, ft	53000
Width, ft	53000
Thickness, ft	1000
Depth at top of formation at injection well, ft	5300
Temperature, °F	140
Initial pressure, psia	2265
Dip, degree	1
Salinity, ppm	100000
Dykstra-Parsons coefficient	0.7
Horizontal to vertical permeability ratio	0.001
Mean permeability, md	100
Horizontal permeabilities of each layer*, md	
Layers 1-4	89
Layers 5-8	65
Layers 9-12	46
Layers 13-16	30
Layers 17-20	15
Layers 21-24	120
Layers 25-28	165
Layers 29-32	235
Layers 33-36	840
Layers 37-40	370
Porosity	0.25
Residual water saturation	0.25
Residual gas saturation	0.25
Gas end point relative permeability	1.0
Water end point relative permeability	0.334
Grid	40×40×40
Maximum injection pressure, psia	3300
Maximum injection rate, MMSCF/D	50

Description of Components

Component	CO_2	H_2O
Critical pressure, psi	1070.0	3200.11
Critical temperature, °F	87.77	705.1
Critical volume, cu ft/lb-mole	1.5076	0.8962
Molecular weight, lb/lb-mole	44.01	18.015
Acentric factor, dimensionless	0.22394	0.344
Parachor, dimensionless	78	52

Mineral	**$Log_{10} K_{sp}$**	**$Log_{10} k_\beta$, mol/m²-s**	**$\hat{A}_\beta$, m²/m³**	**Ea_β, J/mol**
Calcite	1.36	-8.8	88	41870
Anorthite	-8	-12	88	67830
Kaolinite	5.47	-13	17600	62760
Siderite	10.7	-9.35	88	41870
Glauconite	-8.6	-14	4400	58620

Aqueous Species	**Concentration, mol/kg H_2O**
H+	1.0E-7
Ca^{2+}	9.12E-5
$SiO_2(aq)$	2.35E-8
Al^{3+}	2.32E-11
Fe^{2+}	3.22E-6
Fe^{3+}	4.99E-5
Mg^{2+}	5.E-7
K^+	5.E-7
OH^-	5.46E-7
CO_3^{2-}	2.49E-2
HCO_3^-	1.17E-5

Numerical modelling: practical example

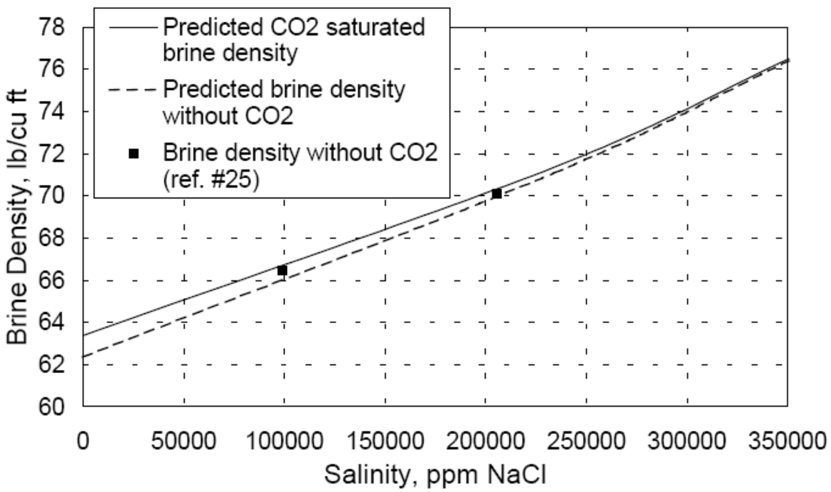
Case 1 - CO_2 injection only	Injection 100 m^3/day of CO_2 for 10 years and shut-in
Case 2 - simultaneous water injection	Co-injection 100 m^3/day of CO_2 and 100 m^3/day of water for 10 years and shut-in
Case 3 - sequential water injection	Sequential injection 100 m^3/day of CO_2 for 10 years, then 100 m^3/day of water for another 10 years and shut-in
Case 4	Increase initial anorthite concentration to 10 times more than that of Case 3

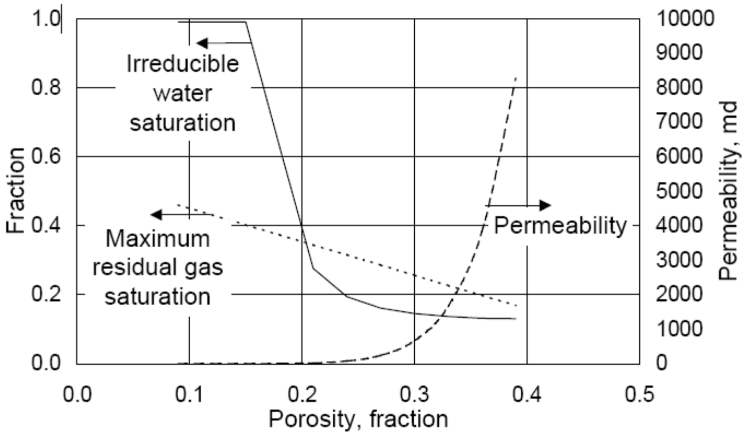
Source	Temperature Range, °F	Pressure Range, psia	Salinity Range, ppm total dissolved solids
15	104-319	100-1400	230,000-350,000
16	120-302	1450-5800	0
18-19	40-69	930-4280	0-31,000

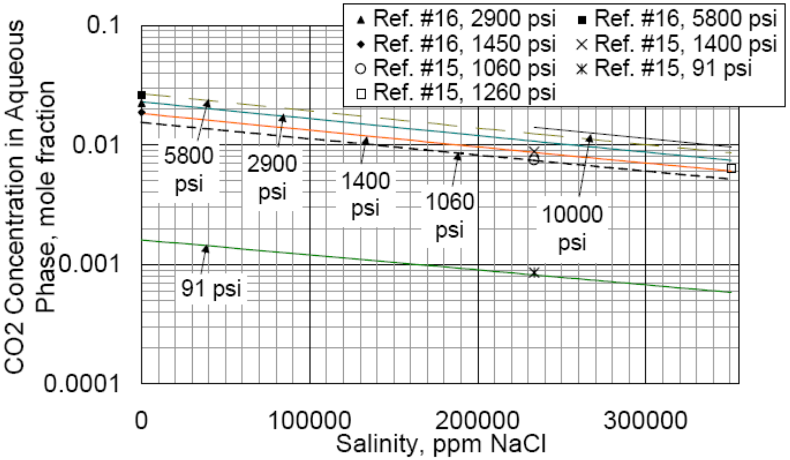
Mineral	Molecular Weight	Density, kg/m^3	Initial Volume Fraction
Calcite	100.1	2710	0.0088
Anorthite	278.2	2740	0.0088
Kaolinite	258.16	2410	0.0176
Siderite	115.86	3960	0.0088
Glauconite	426.93	2670	0.044

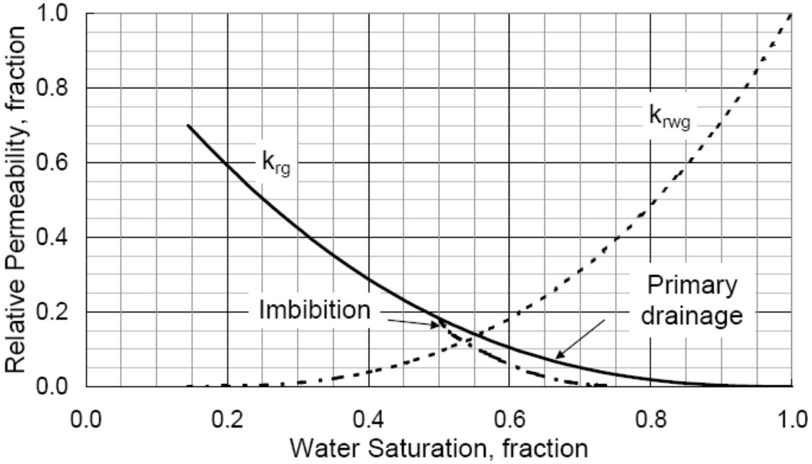
Reaction	Equilibrium Constant, $\log_{10} K$
$H_2O \leftrightarrow H^+ + OH^-$	-13.2631
$CO_2(aq) + H_2O \leftrightarrow H^+ + HCO_3^-$	-6.3221
$CO_2(aq) + H_2O \leftrightarrow 2H^+ + CO_3^{2-}$	-16.5563

Numerical modelling: practical example









Numerical modelling: practical example

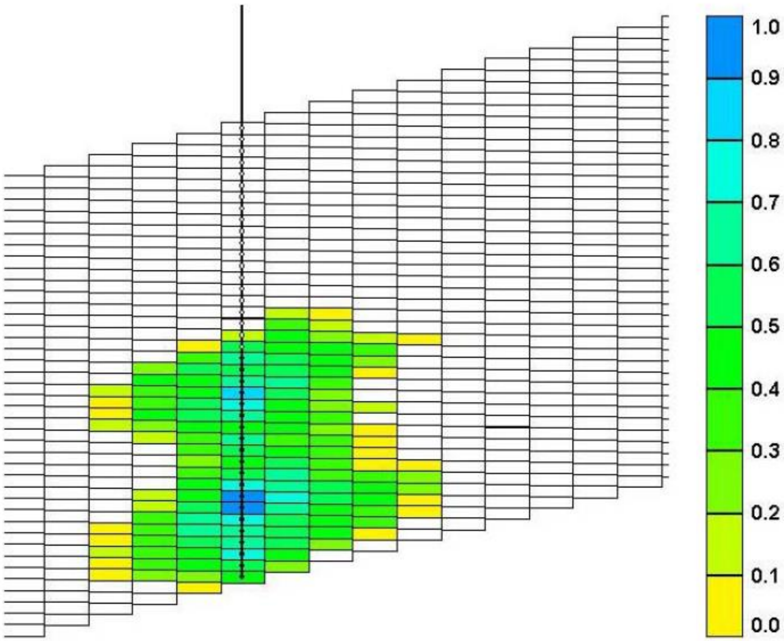


Fig. 7—Gas saturation at 50 years (zoomed-in vertical slice through the injection well in x-z direction)

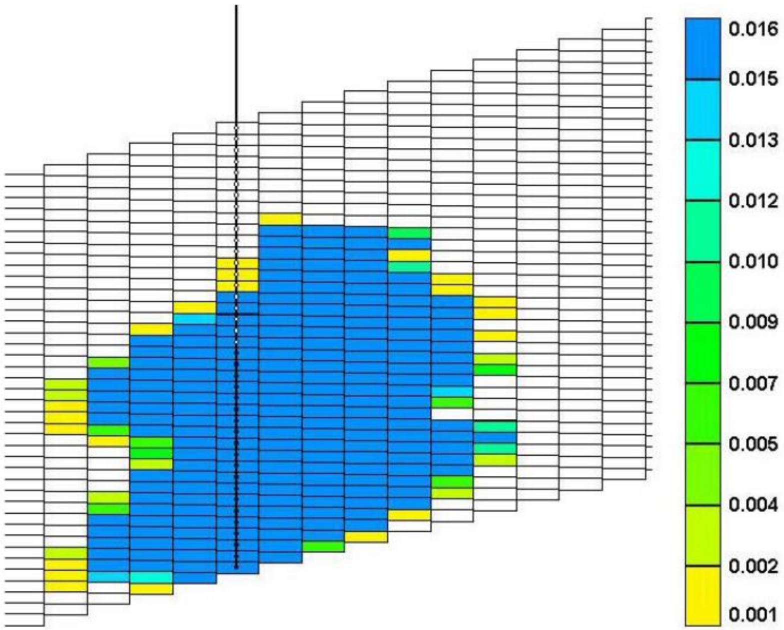


Fig. 9—CO2 mole fraction in aqueous phase at 1000 years (zoomed-in vertical slice through the injection well in x-z direction)

Numerical modelling: practical example

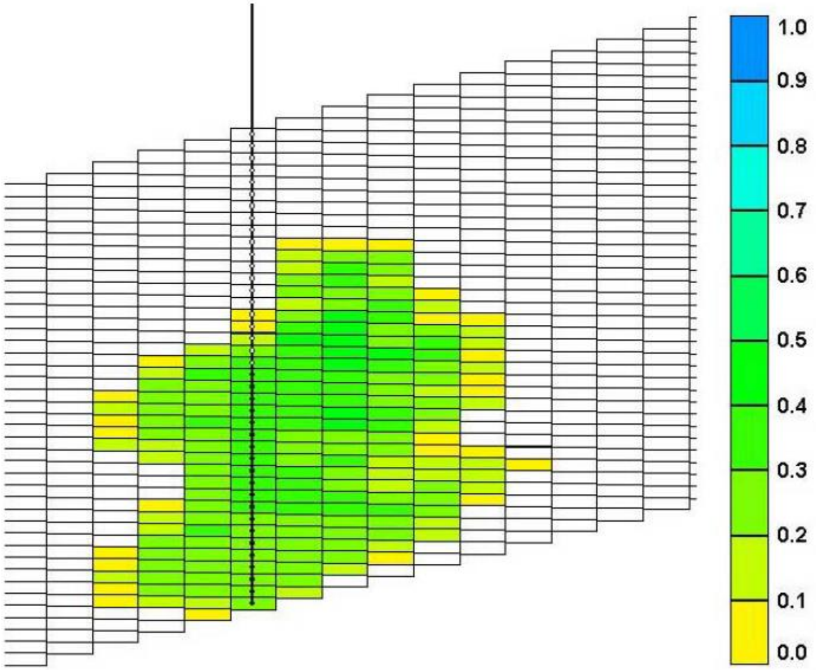


Fig. 8—Gas saturation at 1000 years (zoomed-in vertical slice through the injection well in x-z direction)

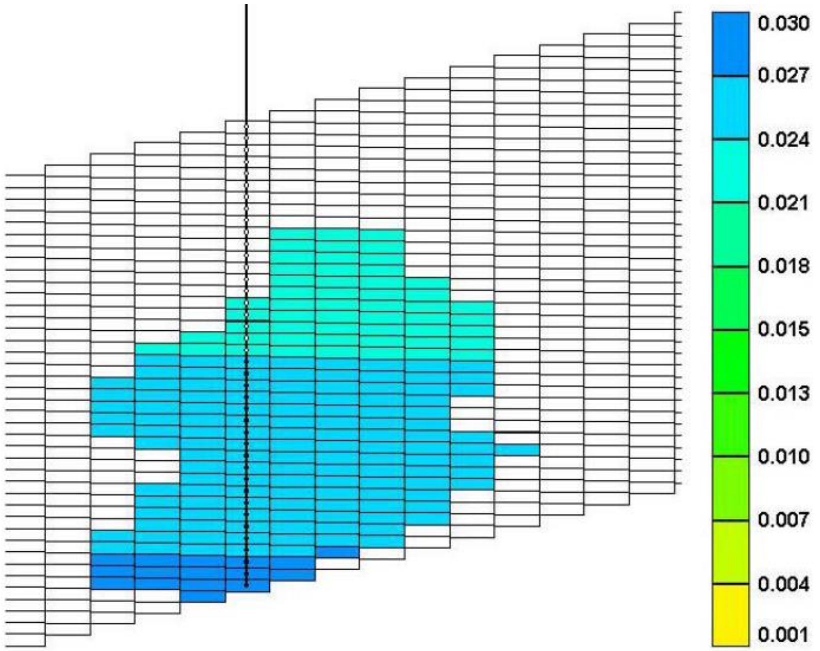


Fig. 10—H_2O mole fraction in gas phase at 1000 years (zoomed-in vertical slice through the injection well in x-z direction)

Numerical modelling: practical example

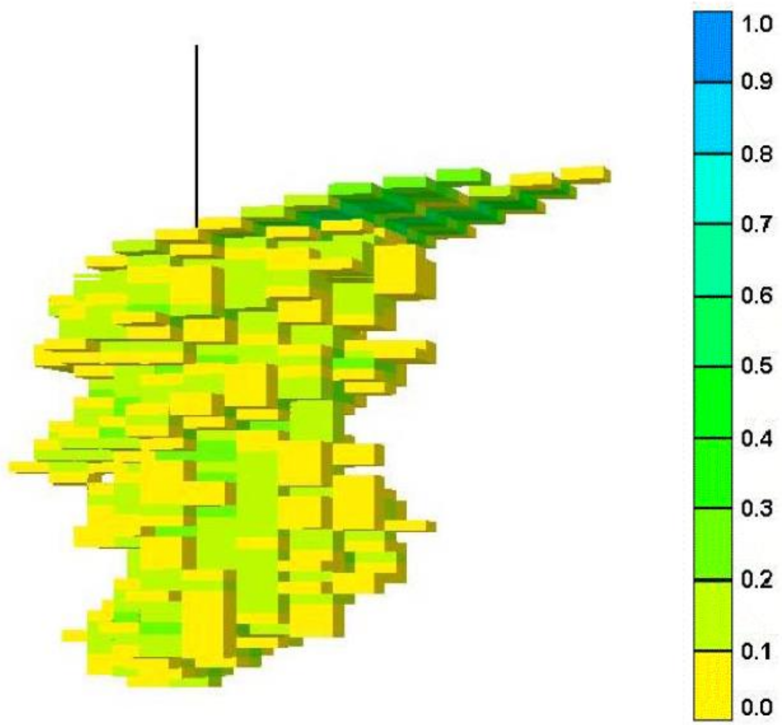


Fig. 12—3-D Gas saturation profile at 1000 years for injection along whole interval

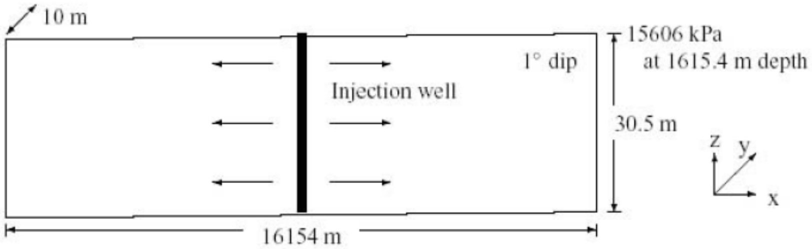


Fig. 13—Schematic of 1D flow field used for simulations that account for mineralization

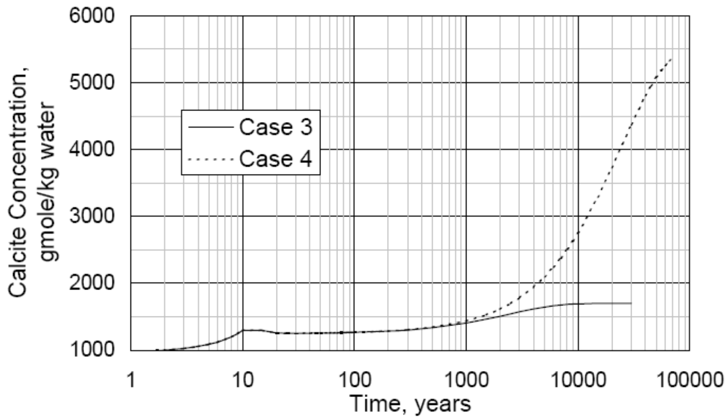


Fig. 16—Comparison of calcite precipitation histories for Case 3 and 4. Case 4 has 10 times more initial anorthite than Case 3

Final thoughts

- Pre-injection dynamic modelling is an important step in the planning and execution of CO2 storage project, particularly in saline aquifers where data are very limited.
- The quality of the input data determines the quality of the results and significant time should be spent on input data quality assurance stages.
- The uncertainty associated with the geologic data is much larger (orders of magnitude) than the difference of results from differences that might exist among the codes used in the modelling.
- Studies suggest that residual saturation trapping is very significant, even more significant than dissolution or mineralization trapping.
- Dynamic reservoir modeling is an excellent tool for sensitivity studies.